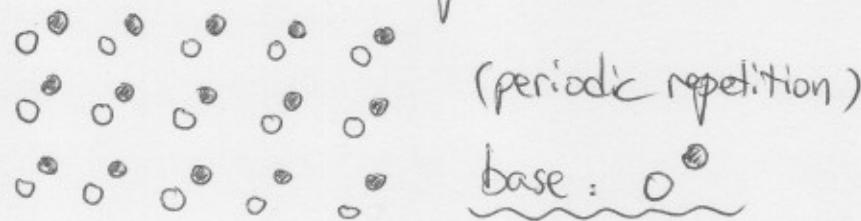


7. Microscale heat conduction

7.1. Basic Concepts of Solids

- * Ideal solid (crystal) — constructed by repetition of identical structural units in space.



- * What holds a crystal together — attractive electrostatic interaction between electrons (- charges) and the nuclei (+ charges). Chemical bonds between atoms in a solid:

Van der Waals (atomic dipole-dipole interaction) ionic bond (oppositely charged ions) Covalent bond (atoms sharing electrons) metallic bond (conducting electrons shared by all atoms) hydrogen bond (hydrogen atom attracted by two atoms)	e.g. Ar-Ar e.g. NaCl e.g. C-C e.g. Cu e.g. H ₂ O
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- * Types of solids.

Single crystals — ideal crystals polycrystals — with single crystal grains (different orientation) Amorphous solids — no "long-range" atomic order
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* Types of solid structures

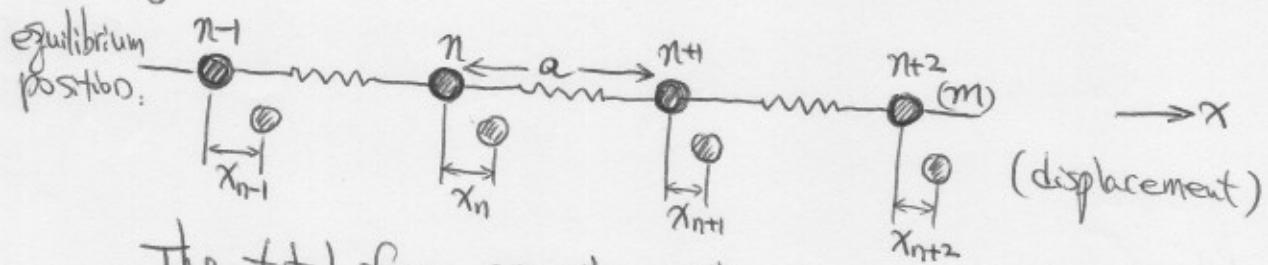
- { "bulk" solids (3D)
- thin films (2D)
- quantum wires (1D) — nanowires
- quantum dots (0D) — nanocrystals

7.2. Phonons in Solids

* A crystal can be considered as an array of atoms attached by "springs" (with force constant C)

7.2.1 Vibrations of crystals with monatomic basis

Consider a one-dimensional array of atoms and springs (1D crystal) shown as.



The total force on the n^{th} atom: (nearest neighbor interaction)

$$F_n = C(x_{n+1} - x_n) + C(x_{n-1} - x_n)$$

The equation of motion of the n^{th} atom:

$$m \frac{d^2 x_n}{dt^2} = C(x_{n+1} + x_{n-1} - 2x_n) \quad (\text{for each atom})$$

Assuming the solution having wave nature:

$$x_n = A e^{i K n a} \cdot e^{-i \omega t}$$

wave vector angular frequency

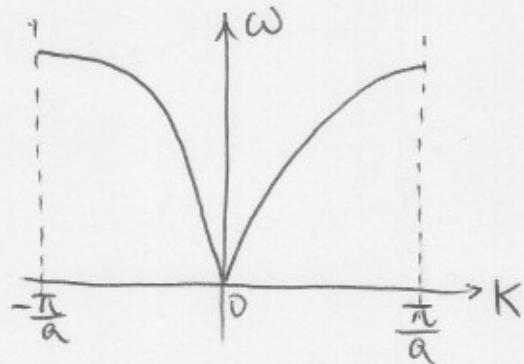
(travelling wave)

Then: $m(-\omega^2)Ae^{ikna} \cdot e^{-i\omega t} = C(Ae^{i(kn+a)} \cdot e^{-i\omega t} + Ae^{i(kn-a)} \cdot e^{-i\omega t} - 2Ae^{ikna} \cdot e^{-i\omega t})$

$$-\omega^2 m = C(e^{ika} + e^{-ika} - 2)$$

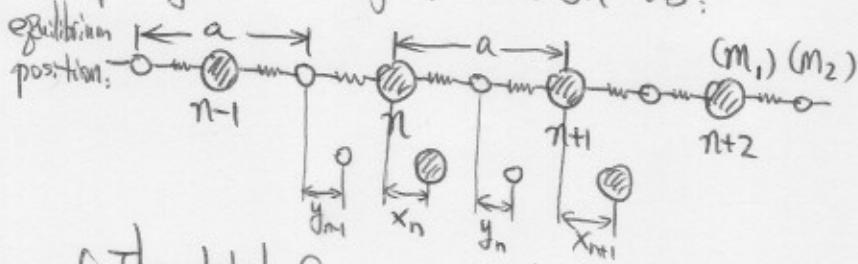
i.e.: $\omega^2 = \frac{2C}{m}(1 - \cos ka)$

or: $\omega = 2\sqrt{\frac{C}{m}} |\sin \frac{ka}{2}|$ dispersion relation.



7.2.2. Vibrations of crystals with two-atom basis

Consider a one-dimensional array of atoms and springs (1D crystal) shown as:



The total force on the n^{th} (M_1) atom:

$$F_{n1} = C(y_n - x_n) + C(y_{n-1} - x_n)$$

The total force on the n^{th} (M_2) atom:

$$F_{n2} = C(x_{n+1} - y_n) + C(x_n - y_n)$$

The equations of motion for n^{th} (m_1) and (m_2) atoms.

$$\left\{ \begin{array}{l} m_1 \frac{d^2x_n}{dt^2} = C(y_n + y_{n+1} - 2x_n) \\ m_2 \frac{d^2y_n}{dt^2} = C(x_n + x_{n+1} - 2y_n) \end{array} \right.$$

Assuming the solution having Wave nature:

$$\left\{ \begin{array}{l} x_n = A e^{ikna} e^{-i\omega t} \\ y_n = B e^{ikna} e^{-i\omega t} \end{array} \right. \quad \begin{array}{l} (\text{different amplitude}) \\ (\text{travelling wave}) \end{array}$$

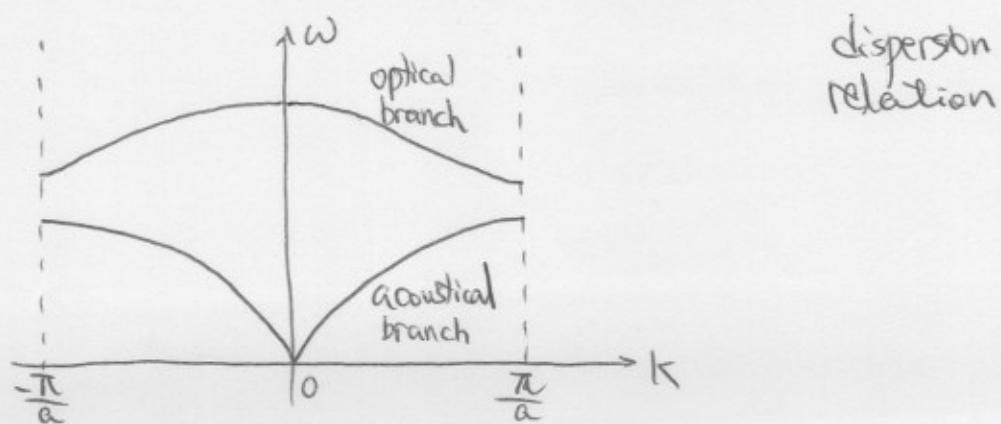
Then: $\left\{ \begin{array}{l} -\omega^2 m_1 A = C \cdot B (1 + e^{-ika}) - 2CA \\ -\omega^2 m_2 B = C \cdot A (1 + e^{ika}) - 2CB \end{array} \right.$

the homogeneous linear equations have a solution only if the determinant of the coefficients vanishes.

$$\begin{vmatrix} 2C - \omega^2 m_1 & -C(1 + e^{-ika}) \\ -C(1 + e^{ika}) & 2C - \omega^2 m_2 \end{vmatrix} = 0$$

i.e.: $m_1 m_2 \omega^4 - 2C(m_1 + m_2)\omega^2 + 2C^2(1 - \cos ka) = 0$

or: $\omega^2 = \frac{C[(m_1 + m_2) \pm \sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos ka}]}{m_1 m_2}$



7.2.3. Phonons.

* Macroscopic view of oscillator energy.

$$U = \frac{1}{2} C x^2$$

energy can be any values
(depending on x)

* Microscopic view of oscillator energy.

$$U = (n + \frac{1}{2}) \hbar \omega$$

$(n = 0, 1, 2, \dots)$

energy takes discrete values
(depending on vibration frequency)
 \hbar is planck constant.

In general, atomic motion in a solid can be transmitted as elastic waves through 3D array of vibrating atom- "spring" network. The elastic waves have different fundamental modes, represented by different vibration frequency, carrying different energy. phonon is the quantum of vibration energy — one quantum of energy in the form of an elastic wave at fixed frequency.

* phonon properties.

① equilibrium distribution of phonons.

$$f_{BE}(\omega) = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

Bose-Einstein distribution

② density of phonon states $D(\omega)$

$D(\omega)$: The number of phonon modes per unit frequency range.

Applying 3D periodic boundary condition for elastic wave

propagation in a solid of volume $V \equiv L_1 L_2 L_3$.

$$\underbrace{e^{i\vec{K} \cdot \vec{r}} = e^{i\vec{K} \cdot (\vec{r} + \vec{L})}}_{(\vec{L} \equiv L_1 \hat{x} + L_2 \hat{y} + L_3 \hat{z})}$$

The periodic B.C. requires \vec{K} (wavevector) to take only discrete values ($\vec{K} \cdot \vec{L} = 2l\pi$):

$$\left\{ \begin{array}{l} K_x = 0, \frac{2\pi}{L_1}, \frac{4\pi}{L_1}, \dots \\ K_y = 0, \frac{2\pi}{L_2}, \frac{4\pi}{L_2}, \dots \\ K_z = 0, \frac{2\pi}{L_3}, \frac{4\pi}{L_3}, \dots \end{array} \right.$$

In \vec{K} -space:

- there is one allowed wavevector \vec{K} per volume $\frac{8\pi^3}{L_1 L_2 L_3} = \frac{8\pi^3}{V}$.
- each \vec{K} takes \vec{K} -space volume $\frac{8\pi^3}{V}$.
- there are $\frac{V}{8\pi^3}$ allowed wavevectors per unit \vec{K} -space volume.
- The total number of \vec{K} modes with wavevector smaller than K is:

$$N_{(<K)} = \underbrace{\frac{4}{3}\pi K^3}_{\text{R-space volume}} \cdot \left(\frac{V}{8\pi^3}\right)$$

- the density of states

$$D(\omega) = \underbrace{\frac{dN_{(<K)}}{d\omega}}_{\text{depending on dispersion relation}} = \frac{VK^2}{2\pi^2} \frac{dK}{d\omega}$$

7.24. phonon heat capacity of Solids

The thermal energy of solid (phonon contribution) is.

$$U = \sum_{\vec{K}} \sum_p \frac{\hbar \omega_p(\vec{K})}{e^{\frac{\hbar \omega_p(\vec{K})}{k_B T}} - 1}$$

$$= \sum_p \int D_p(\omega) \frac{\hbar \omega}{e^{\frac{\hbar \omega}{k_B T}} - 1} d\omega$$

↑
polarization

Debye model: $\omega = v k$ (acoustical dispersion relation)

$$\text{so: } D(\omega) = \underbrace{\frac{\omega^2 V}{2\pi^2 v^3}}$$

$$U = 3 \times \int_0^{w_D} \frac{\omega^2 V}{2\pi^2 v^3} \frac{\hbar \omega}{e^{\frac{\hbar \omega}{k_B T}} - 1} d\omega$$

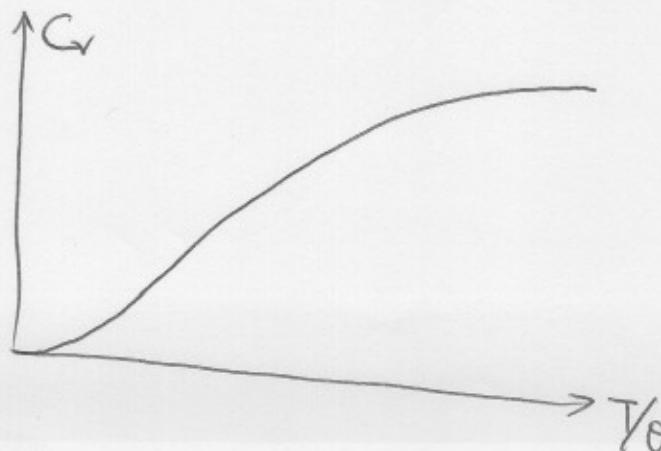
3 polarization in 3D
for acoustical modes

Note: assuming there are N
unit cells in solid,
so N acoustical modes.
A cut-off frequency
is determined by:
 $w_D = \left(\frac{6\pi^2 v^3 N}{V} \right)^{1/3}$

$$\text{so: } U = 9Nk_B T \left(\frac{T}{\theta} \right)^3 \int_0^{\theta} \frac{x^3}{e^x - 1} dx$$

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V = 9Nk_B \left(\frac{T}{\theta} \right)^3 \int_0^{\theta} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

$$\theta = \frac{\pi v}{k_B} \left(\frac{6\pi^2 N}{V} \right)^{1/3}$$



at low T ($T \ll \theta$),
 $C \propto T^3$